

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 7.40×10^{-11} cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 6.47×10^{-2}

Confidence level: 8.07×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Myrcene

Measured: 2.15×10^{-10}

Predicted: 2.05×10^{-10}

Image not found

2-Methyl-p-benzoquinone

Measured: 2.35×10^{-11}

Predicted: 2.15×10^{-11}